Quantum Effects in de Sitter and Anti-de Sitter Spaces

Applications to Diatomic Molecules

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Overview

- General Introduction
- Nikiforov–Uvarov Method
- Validation via Numerical Solver
- Pseudo-Harmonic Potential
- Kratzer Potential
- Critical Parameters (λ_c, λ_f)
- Applications and Conclusion

General Introduction

1 Introduction

- Quantum mechanics describes microscopic systems
- Schrödinger equation governs bound states
- Diatomic molecules: key systems in spectroscopy
- Importance in quantum technologies
- Study extended to curved space-time

Motivation

- Analytical solutions difficult in curved spaces
- Need for generalized method
- Study deformation effects on energy spectra
- Link with quantum computing

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2 Nikiforov–Uvarov Method

General Equation

2 Nikiforov–Uvarov Method

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0$$

- $\sigma(s)$: polynomial of degree 2
- $\tilde{\tau}(s)$: degree 1
- $\tilde{\sigma}(s)$: degree 2

Polynomial Structure

2 Nikiforov–Uvarov Method

$$\pi(s) = As + B \pm \sqrt{\cdots}$$

- Determines wavefunction behavior
- Two possible solutions
- Physical condition: $\tau'(s) < 0$

Eigenvalues

2 Nikiforov–Uvarov Method

$$\lambda_n = n\left(2\sqrt{A^2+\xi_1+k\alpha_3}+\alpha_2-2A\right)-\frac{n(n-1)\alpha_3}{2}$$

- Provides energy spectrum
- Depends on deformation parameter

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3 Pseudo-Harmonic Potential

Potential

3 Pseudo-Harmonic Potential

$$V(r) = D_e \left(\frac{r}{r_e} - \frac{r_e}{r} \right)^2$$

- Models molecular vibrations
- Includes anharmonic effects

Transformation

3 Pseudo-Harmonic Potential

$$y = \sqrt{1 + k\lambda r^2}$$

- Reduces equation to NU form
- Allows exact solution

Energy Spectrum

3 Pseudo-Harmonic Potential

$$E_{n,l,\kappa} = \hbar\sqrt{\frac{2D_e}{mr_e^2}}\sqrt{1+\frac{\lambda^2\hbar^2 r_e^2}{8mD_e}}\left(2n+\sqrt{\left(l+\tfrac{1}{2}\right)^2+\frac{2mD_e r_e^2}{\hbar^2}}+1\right) - \frac{\lambda\kappa\hbar^2}{m}\left[\left(n+\tfrac{1}{2}\right)\left(2n+2\sqrt{\left(l+\tfrac{1}{2}\right)^2+\frac{2mD_e r_e^2}{\hbar^2}}+1\right)-\tfrac{1}{4}\right]-2D_e.$$

$$E_{n,l} = f(n,l,\lambda)$$

- Depends on deformation
- Non-uniform shift of levels

Physical Interpretation

- dS ($k = +1$): stronger confinement
- AdS ($k = -1$): weaker binding
- Possible level inversion

Critical λ_f Values

3 Pseudo-Harmonic Potential

Molecule	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$
CaF ($n = 1$)	0.06897				
CaF ($n = 2$)	0.09536	0.19072			
CaF ($n = 3$)	0.12175	0.24350	0.36525		
BaH ($n = 1$)	0.09154				
BaH ($n = 2$)	0.12667	0.25334			
BaH ($n = 3$)	0.16180	0.32360	0.48540		

They indicate thresholds where energy levels may invert.

Energy Levels for CaF

3 Pseudo-Harmonic Potential

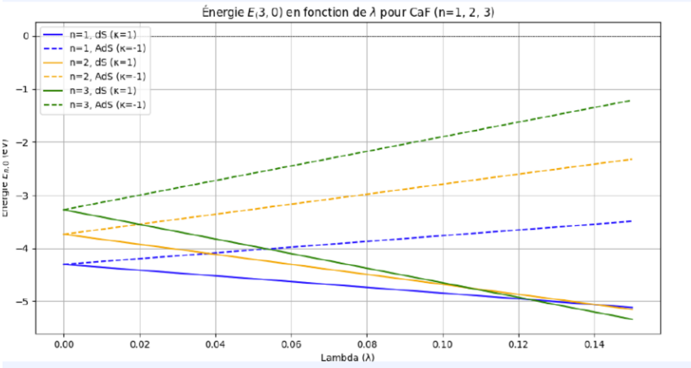

Figure: PHO energy spectrum for CaF in dS and AdS spaces

- The deformation parameter λ strongly modifies the energy spectrum
- In de Sitter space ($k = +1$): energy decreases as λ increases → stronger binding
- In Anti-de Sitter space ($k = -1$): energy increases toward zero → weaker binding and possible ionization
- Higher excited states ($n = 3$) are more sensitive to deformation effects
- This behavior indicates a non-uniform deformation impact across quantum states

Energy Levels for BaH

3 Pseudo-Harmonic Potential

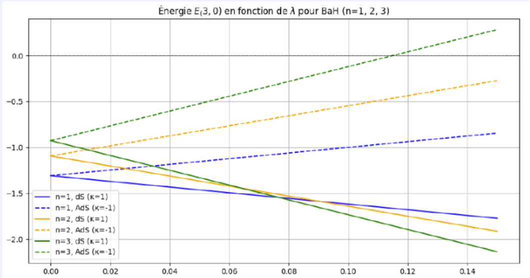

Figure: PHO Energy for BaH in both dS and AdS spaces

- Similar trends are observed.
- Strong dependence on n

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4 Kratzer Potential

Kratzer Potential

$$V(r) = D_e \left(\frac{r - r_e}{r} \right)^2$$

- Describes molecular bonding
- Includes Coulomb-like term

Transformation

4 Kratzer Potential

$$s = \frac{\sqrt{1 + k\lambda r^2}}{\sqrt{k\lambda r^2}}$$

- Leads to solvable NU equation

Energy Spectrum

4 Kratzer Potential

$$
\begin{aligned}
E_{n,l} = & -\frac{4mD_e^2 r_e^2}{2\hbar^2}\left(n+\tfrac{1}{2}+\sqrt{\left(l+\tfrac{1}{2}\right)^2+\tfrac{2mD_e r_e^2}{\hbar^2}}\right)^{-2} \\
& -\frac{\kappa\lambda\hbar^2}{2m}\left[\left(n+\tfrac{1}{2}+\sqrt{\left(l+\tfrac{1}{2}\right)^2+\tfrac{2mD_e r_e^2}{\hbar^2}}\right)^2-\left(\left(l+\tfrac{1}{2}\right)^2+\tfrac{2mD_e r_e^2}{\hbar^2}\right)-\tfrac{3}{4}\right].
\end{aligned}
$$

$$E_{n,l} = f(n, l, \lambda)$$

- Modified by deformation
- Strong curvature effects

Physical Interpretation

4 Kratzer Potential

- AdS: weaker binding
- dS: stronger confinement
- Critical $\lambda_c \rightarrow$ ionization threshold

Critical Deformation Parameter λ_c

4 Kratzer Potential

Analytical Expression

$$\lambda_c(n,l) = \frac{m^2 \left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2mD_e r_e^2}{\hbar^2}}\right)^{-2}}{\hbar^4 \left[\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2mD_e r_e^2}{\hbar^2}}\right)^2 - \left(\left(l + \frac{1}{2}\right)^2 + \frac{2mD_e r_e^2}{\hbar^2}\right) - \frac{3}{4}\right]}$$

- λ_c corresponds to the value where the bound-state energy vanishes: $E_{n,l} = 0$
- It defines the ionization threshold of the molecule
- Strong dependence on quantum numbers (n, l) and molecular parameters

Kratzer Potential: Energy Levels for CaF

4 Kratzer Potential

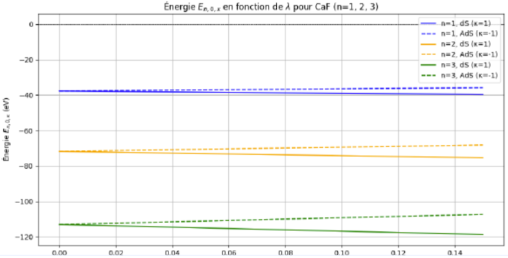

Figure: Kratzer energy spectrum for CaF in dS and AdS spaces

- Energy levels are strongly affected by the deformation parameter λ
- In AdS space ($k = -1$): energy increases toward zero → weaker binding
- In dS space ($k = +1$): energy decreases → stronger confinement
- The effect is more pronounced for higher quantum numbers

Kratzer Potential: Energy Levels for BaH

4 Kratzer Potential

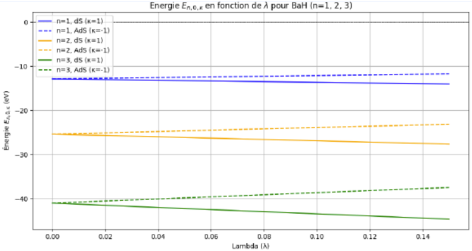

Figure: Kratzer energy spectrum for BaH in dS and AdS spaces

- Similar deformation behavior is observed for BaH molecule
- Energy levels shift non-uniformly with λ
- Higher excited states are more sensitive to deformation
- Comparison with CaF shows molecular dependence of deformation effects

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5 Applications

Quantum Technology Implications

5 Applications

- Deformation affects energy spacing
- Level inversion impacts stability
- CaF and BaH as molecular qubits
- Tunable quantum transitions

Toward Experimentation

5 Applications

- Optical lattices simulate curvature
- Cold atoms mimic quantum systems
- Spectroscopy detects deformation

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6 Conclusion

Conclusion

6 Conclusion

- NU method provides analytical solutions
- Deformation modifies spectra
- PHO and Kratzer successfully solved
- Applications in quantum computing

Outlook

6 Conclusion

- Extend to Morse and Hulthén potentials
- Include relativistic effects
- Study time-dependent deformation
- Quantum technology applications